Exploration of Multi-dimensional Density of States by Multicanonical Monte Carlo algorithm

Yukito IBA[1,*] and Hisanao TAKAHASHI[2]

[1] *The Institute of Statistical Mathematics, Tokyo 106-8569, Japan*
[2] *267-5 Kita-Akitsu Tokorozawa-shi Saitama-ken 359-0038, Japan*

Multi-dimensional density of states provides a useful description of complex frustrated systems. Recent advances in Monte Carlo methods enable efficient calculation of the density of states and related quantities, which renew the interest in them. Here we calculate density of states on the plane (energy, magnetization) for an Ising Model with three-spin interactions on a random sparse network, which is a system of current interest both in physics of glassy systems and in the theory of error-correcting codes. Multicanonical Monte Carlo algorithm is successfully applied, and the shape of densities and its dependence on the degree of frustration is revealed. Efficiency of multicanonical Monte Carlo is also discussed with the shape of a projection of the distribution simulated by the algorithm.

§1. Introduction

Given a system of the energy $E(\boldsymbol{x})$, the density of states of physical quantities $A_0(\boldsymbol{x}), A_1(\boldsymbol{x}), \ldots$ is defined as

$$D(A_0 = a_0,\, A_1 = a_1,\, \ldots) \,=\, \sum_{\boldsymbol{x}} \,\Big\{ \delta(A_0(\boldsymbol{x}) - a_0) \times \delta(A_1(\boldsymbol{x}) - a_1) \times \cdots \Big\},$$

where δ is defined as usual: $\delta(a) = 1$ if $a = 0$, else $\delta(a) = 0$. Usually, one of the A_is' is the energy $E(\boldsymbol{x})$ itself. When we set $A_0(\boldsymbol{x}) = E(\boldsymbol{x})$ and ignore other A_is', it gives the original definition of a univariate "density of state" $D(E)$, which is the normalization constant of microcanonical distribution $P^{mc}(\boldsymbol{x}) = \delta(E(\boldsymbol{x}) - E_0)/D(E_0)$. Hereafter we are mostly interested in bivariate cases where $A_0(\boldsymbol{x}) = E(\boldsymbol{x})$, $A_1(\boldsymbol{x}) = M(\boldsymbol{x})$, where $M(\boldsymbol{x})$ is an order parameter of a system, for example, magnetization of an Ising ferromagnet.

Recently, an introduction of extended Monte Carlo methods,[1)] especially multicanonical Monte Carlo algorithm,[1)–3)] makes calculation of multi-dimensional densities of states a realistic choice for the analysis of complex probability distributions. There is a special interest in studying the cases with a first-order transition with latent heat with this approach. Existence of the latent heat indicates a rapid drop of the entropy of the system in ordering and suggests the difficulty in searching ground states. It will be interesting to investigate the nature of ordering process through the calculation of the multi-dimensional density of states. In this paper we study Ising models with three-spin interactions on random sparse networks ("Sourlas code")[4)] and calculate density of the states and related quantities by multicanonical Monte Carlo.

*) E-mail: iba@ism.ac.jp

§2. Multicanonical Monte Carlo

Details of multicanonical Monte Carlo algorithm are found in the references.[1),2)] The essence of the algorithm is dynamical Monte Carlo sampling with a weight $1/\tilde{D}(E)$, where $\tilde{D}(E)$ is an approximation of $D(E)$. It causes a nearly uniform distribution of the energy E within an interval. The density $\tilde{D}(E)$ is estimated by repeated "preliminary runs" of the simulation (a simple method called "entropic sampling"[5)] is used here). The bivariate density $D(E, M)$ is obtained by $\log D(E, M) = \log W(E, M) + \log(\tilde{D}(E)) + const.$, where $W(E, M)$ is the frequencies of the values (E, M) appeared in a simulation with the weight $1/\tilde{D}(E)$. We can also reconstruct a conditional density $D(M|E)$ by $\log D(M|E) = \log D(E, M) - \sum_M \log D(E, M)$. $D(E|M)$ is proportional to the projection on (E, M) plane of the distribution sampled by multicanonical Monte Carlo with an ideal weight $\tilde{D}(E) = D(E)$.

The advantage of multicanonical Monte Carlo is that relaxation in small E (and also very high E) region is greatly facilitated compared with canonical or microcanonical simulations. An interesting question is when multicanonical Monte Carlo performs better than the other methods with extended ensembles, parallel tempering[1)] and simulated tempering.[1),6)] It is usually believed that multicanonical Monte Carlo performs better in cases with first-order transitions with latent heat, because multicanonical ensemble can contain states that rarely appear in a canonical distribution of any temperature, and relaxation is speed up with a vanishing critical nucleus size. This picture, however, seems not to be tested enough. We will discuss it in the later section with our example.

§3. Ising Model with three-spin interactions

Let us consider an Ising model with three-spin interactions:

$$P_\beta(\boldsymbol{x}) \propto \exp\left(\beta \sum_{(ijk)\in G} J_{ijk} x_i x_j x_k\right).$$

Here $\sum_{(ijk)\in G}$ denotes the summation on the edges of a graph G. The energy and the magnetization is defined as $E = \sum_{(ijk)\in G} J_{ijk} x_i x_j x_k$, and $M = \sum_i x_i$, respectively. Several different definitions of a random network G is possible. Here we consider a simplest case to simulate: The probability of the presence of the edge is independent and takes the same value for all pairs of the vertices on G. Total number of edges are fixed to a given number I, but the number K of the edges that contains a vertex is not fixed. Hereafter we set $J_{ijk} = \pm 1$.

An example of the results are shown in Figs. 1 and 2 for a ferromagnetic model ($J_{ijk} \equiv 1$) of the size $N = 100$ on a random graph G with $I = 200$ edges. Density of states $D(E, M)$ and the projection $D(E|M)$ of multicanonical density are plotted in Figs. 1 and 2. The vertical and horizontal axes corresponds to the energy E and the magnetization M. In Figs. 1 and 2, an interval of the contours corresponds to the change of the density by the factors 10^4 and $10^{0.5} \sim 3.2$, respectively.

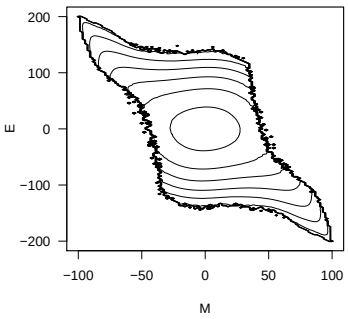

Fig. 1. Density of States: $\log D(E, M)$

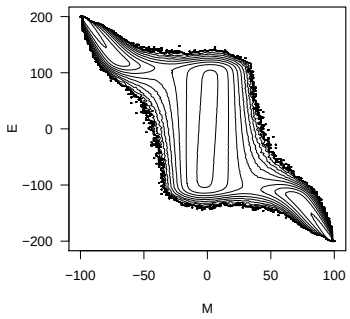

Fig. 2. Multicanonical Density: $\log D(M|E)$

In Fig. 1, states around $(E, M) = \pm(200, 100)$ at the ends of "arm"s observed in both sides of the body correspond to the ordered states, while the peak at the center corresponds to the paramagnetic state. Point symmetry of the density corresponds to $S_i \to -S_i$, $(E, M) \to (-E, -M)$ symmetry of the model. In Fig. 2, three peaks of the density are observed, one of which is the paramagnetic state at the center, and the others correspond to ordered states. Multiple peaks indicate that metastabilty appears even with multicanonical Monte Carlo.

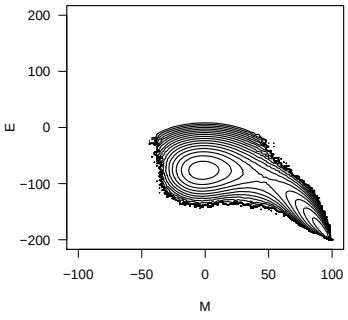

Fig. 3. Distribution of (E, M) at $\beta = 0.4$.

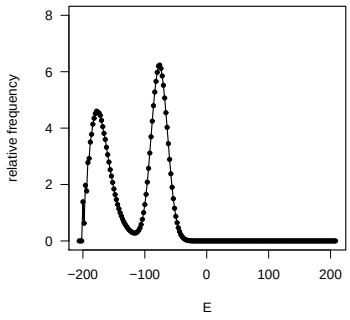

Fig. 4. Distribution of E at $\beta = 0.4$.

In Figs. 3 and 4, projections of a canonical distribution $P_\beta(x)$ ($\beta = 0.4$) on the (E, M) plane and on the E plane are shown, respectively. In Fig. 3, the contour interval and axes are the same as those in Fig. 2. Two peaks are again seen in both figures, which agree with an existence of the first-order transition with latent heat.[4)]

The changes of the shape of density of states when we add frustration are shown in Figs. 5-7. Models with $N = 100$ and $I = 500$ are investigated for the ratio p of negative bonds 0, 0.1, and 0.36. The contour interval and axes are the same as those in Fig. 1. Increasing the concentration of frustration, the maximum value of magnetization that appears with a probability higher than a threshold reduces and the "arm"s shrink. At the value $p = 0.36$, there are no more evident arms, which indicate ordered states do not exist at any temperature.

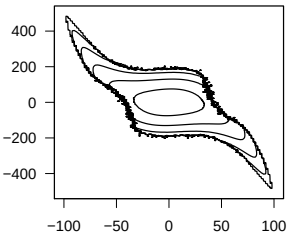

Fig. 5. $p = 0$

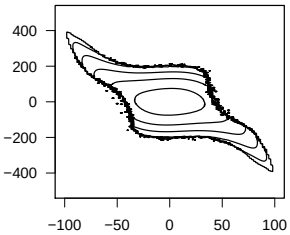

Fig. 6. $p = 0.1$

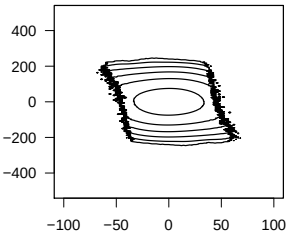

Fig. 7. $p = 0.36$

For each of these examples, $1.0 \sim 1.5 \times 10^9$ MCS are required for the estimation of $\tilde{D}(E)$ and $\sim 10^8$ MCS are used for the computation of the physical quantities. Typical CPU times are $10 \sim 15$ hours with a 3.2GHz Pentium4 chip.

§4. Discussion and Future Problems

The result shown in Fig. 2 give rise to the possibility that (univariate) multicanonical Monte Carlo may not have a clear advantage over parallel tempering in this example. A natural question is that how multicanonical density looks like for other systems with first-order transition with latent heat. Our preliminary results on 10-states Potts model on the square lattice indicate that multicanonical density projected on a (energy, order parameter) plane shows smoother behavior compare with those of Ising models with three-spin interactions, although a saddle point is still observed. Detailed comparison is, however, left for future studies, as well as computation of a thermodynamic limit of the densities and direct comparison between multicanonical and parallel tempering algorithm.

Another interesting issue is the use of two-dimensional multicanonical Monte Carlo[3] with the weight $1/\tilde{D}(E, M)$ that approximates inverse of the bivariate density $D(E, M)$. It enables efficient sampling of small $D(E, M)$ regions, and, hopefully, further enhance the mixing. Our experience, however, shows that it requires considerably many iterations for the estimate of the bivariate $\tilde{D}(E, M)$ by entropic sampling. Some improvements in the learning stage should be introduced in future studies.

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